

Appendix A

Data Assimilation

A.1 Derivation of the Euler-Lagrange Equations

This Section outlines the derivation of the Euler-Lagrange equations presented in Section 2.1.3. In order to find the minimum of the objective function, we perform a first variation on J .

$$\delta J = \frac{\delta J}{\delta X} \delta X + \frac{\delta J}{\delta Y} \delta Y + \frac{\delta J}{\delta \nu} \delta \nu + \frac{\delta J}{\delta \omega} \delta \omega + \frac{\partial J}{\partial \alpha} \delta \alpha + \frac{\partial J}{\partial \beta} \delta \beta + \frac{\delta J}{\delta \mu} \delta \mu + \frac{\delta J}{\delta \lambda} \delta \lambda + \frac{\partial J}{\partial \lambda_0} \delta \lambda_0 \quad (\text{A.1})$$

At the minimum we have $\delta J = 0$. Since all variations are considered arbitrary and independent, each of the individual partial derivatives of the objective function must vanish.

Obviously, variation of (2.7) with respect to the adjoint parameters μ , λ and λ_0 simply returns the state equation, i.e. the forward equation (2.8) and its initial condition (2.8b) in the set of Euler-Lagrange equations.

From the variation of (2.7) with respect to the parameters α and β , we get

$$\left[2(\alpha - \bar{\alpha})^T C_\alpha^{-1} - 2 \int_0^{t_f} \mu^T \frac{\partial \phi}{\partial \alpha} dt - 2 \int_0^{t_f} \lambda^T \frac{\partial \varphi}{\partial \alpha} dt \right] \delta \alpha = 0$$

and

$$\left[2(\beta - \bar{\beta})^T C_\beta^{-1} - 2\lambda_0^T \frac{\partial Y_0}{\partial \beta} \right] \delta \beta = 0$$

Using $\lambda_0 = \lambda|_{t=0}$ (see below), these are the parameter update equations (2.10).

Next, variation of (2.7) with respect to ω yields

$$2 \int_0^{t_f} \left[\int_0^{t_f} \omega(t')^T C_\omega^{-1}(t', t'') dt' - \lambda(t'')^T D_\omega(t'') P_\omega \right] \delta \omega(t'') dt'' = 0$$

and therefore

$$\int_0^{t_f} \omega(t')^T C_\omega^{-1}(t', t'') dt' = \lambda(t'')^T D_\omega(t'') P_\omega$$

Postmultiplying by $C_\omega(t'', t)$, integrating over t'' , and using (2.6), we find

$$\omega(t)^T = \int_0^{t_f} \lambda(t'')^T D_\omega(t'') P_\omega C_\omega(t'', t) dt''$$

which is the process noise update (2.11a). Similarly, we get the update equation for ν .

Variation with respect to X yields

$$-2(Z - M[X, Y])^T C_v^{-1} \frac{\partial M[X, Y]}{\partial X} \delta X - 2 \int_0^{t_f} \mu^T \frac{\partial \phi}{\partial X} \delta X dt - 2 \int_0^{t_f} \lambda^T \frac{\partial \varphi}{\partial X} \delta X dt = 0$$

In this expression, we substitute from (2.3)

$$\frac{\partial M[X, Y]}{\partial X} = \int_0^{t_f} [\delta] \frac{\partial f(X(t), Y(t))}{\partial X} dt$$

and get the first part of the backward equation after collecting all terms under a single integral and setting the integrand to zero.

In order to perform the variation with respect to the state Y , we start from (2.7) and integrate by parts the term containing $\frac{\partial Y}{\partial t}$.

$$\begin{aligned} J &= (Z - M[X, Y])^T C_v^{-1} (Z - M[X, Y]) \\ &\quad + (\alpha - \bar{\alpha})^T C_\alpha^{-1} (\alpha - \bar{\alpha}) + (\beta - \bar{\beta})^T C_\beta^{-1} (\beta - \bar{\beta}) \\ &\quad + \int_0^{t_f} \int_0^{t_f} \nu(t')^T C_\nu^{-1}(t', t'') \nu(t'') dt' dt'' + \int_0^{t_f} \int_0^{t_f} \omega(t')^T C_\omega^{-1}(t', t'') \omega(t'') dt' dt'' \\ &\quad - 2 \int_0^{t_f} \mu^T (\phi(X, Y; \alpha) + D_\nu P_\nu \nu) dt \\ &\quad + 2 (\lambda^T Y) |_{t=t_f} - 2 (\lambda^T Y) |_{t=0} - 2 \int_0^{t_f} \left(\frac{\partial \lambda^T}{\partial t} Y + \lambda^T \varphi(X, Y; \alpha) + \lambda^T D_\omega(Y) P_\omega \omega \right) dt \\ &\quad + 2 \lambda_0^T (Y|_{t=0} - Y_0(\beta)) \end{aligned}$$

From the variation with respect to $Y|_{t=t_f}$ we immediately get the terminal condition (2.9a) for the backward equation. (Recall that $t_m \in (0, t_f)$, i.e. there are no measurements at the final time t_f). Similarly, variation with respect to $Y|_{t=0}$ yields

$$\lambda|_{t=0} = \lambda_0$$

Finally, variation with respect to the state $Y(t)$, $t \in (0, t_f)$, yields

$$\begin{aligned} &-2(Z - M[X, Y])^T C_v^{-1} \frac{\partial M[X, Y]}{\partial Y} \delta Y \\ &\quad - 2 \int_0^{t_f} \mu^T \frac{\partial \phi}{\partial Y} \delta Y dt - 2 \int_0^{t_f} \left[\frac{\partial \lambda^T}{\partial t} + \lambda^T \frac{\partial \varphi}{\partial Y} + \lambda^T \frac{\partial [D_\omega(Y) P_\omega \omega]}{\partial Y} \right] \delta Y dt = 0 \end{aligned}$$

In this expression, we substitute from (2.3)

$$\frac{\partial M[X, Y]}{\partial Y} = \int_0^{t_f} [\delta] \frac{\partial f(X(t), Y(t))}{\partial Y} dt$$

and get the backward equation after collecting all terms under a single integral and setting the integrand to zero.

A.2 Derivation of the Posterior Covariance Equations

This Section outlines the derivation of the posterior covariance equations of Section 2.4. Recall that the problem at hand is nonlinear, and that the linearized posterior covariances derived below are at best approximations of the true posterior covariances. In particular, we treat the previous estimate as a fixed deterministic input, although strictly speaking the previous estimate depends on the data and therefore on the measurement error.

A.2.1 Equivalence of Representers and Prior Cross-Covariances

We first prove the fact that the state representers are equal to the linearized (prior) cross-covariances of the measurement predictions and the states.

$$\overline{L_k[X', Y']X'(t)} = \Xi^k(t) \quad \overline{L_k[X', Y']Y'(t)} = \Upsilon^k(t) \quad (2.34)$$

The idea is to show that $\overline{L_k[X', Y']X'(t)}$ and $\overline{L_k[X', Y']Y'(t)}$ obey the same differential equations as $\Xi^k(t)$ and $\Upsilon^k(t)$, which are of course the state representer equations (2.25).

From the tangent-linear state equation (2.13) and the equation for the prior state (2.22), we obtain an equation for the perturbation of the state $X' \equiv X - \bar{X}^{\eta+1}$ and $Y' \equiv Y - \bar{Y}^{\eta+1}$.

$$\begin{aligned} 0 &= \frac{\partial \phi}{\partial X} \Big|_{\eta} X' + \frac{\partial \phi}{\partial Y} \Big|_{\eta} Y' + \frac{\partial \phi}{\partial \alpha} \Big|_{\eta} \alpha' + D_{\nu} P_{\nu} \nu \\ \frac{\partial Y'}{\partial t} &= \frac{\partial \varphi}{\partial X} \Big|_{\eta} X' + \frac{\partial \varphi}{\partial Y} \Big|_{\eta} Y' + \frac{\partial \varphi}{\partial \alpha} \Big|_{\eta} \alpha' + D_{\omega}(Y^{\eta}) P_{\omega} \omega + \frac{\partial [D_{\omega}(Y) P_{\omega} \omega]}{\partial Y} \Big|_{\eta} Y' \end{aligned} \quad (A.2)$$

$$Y'|_{t=0} = \frac{\partial Y_0}{\partial \beta} \Big|_{\eta} \beta' \quad (A.2a)$$

For the perturbations of the parameters we write $\alpha' \equiv \alpha - \bar{\alpha}$ and $\beta' \equiv \beta - \bar{\beta}$.

Next, we multiply (A.2) with the scalar $L_k[X', Y']$ and take the expectation. We get

$$\begin{aligned} 0 &= \frac{\partial \phi}{\partial X} \Big|_{\eta} \overline{L_k[X', Y']X'(t)} + \frac{\partial \phi}{\partial Y} \Big|_{\eta} \overline{L_k[X', Y']Y'(t)} + \frac{\partial \phi}{\partial \alpha} \Big|_{\eta} \overline{L_k[X', Y']\alpha'} \\ &\quad + \overline{L_k[X', Y']D_{\nu} P_{\nu} \nu} \\ \frac{\partial}{\partial t} \overline{L_k[X', Y']Y'(t)} &= \frac{\partial \varphi}{\partial X} \Big|_{\eta} \overline{L_k[X', Y']X'(t)} + \frac{\partial \varphi}{\partial Y} \Big|_{\eta} \overline{L_k[X', Y']Y'(t)} + \frac{\partial \varphi}{\partial \alpha} \Big|_{\eta} \overline{L_k[X', Y']\alpha'} \\ &\quad + \overline{L_k[X', Y']D_{\omega}(Y^{\eta}) P_{\omega} \omega} + \overline{L_k[X', Y'] \frac{\partial [D_{\omega}(Y) P_{\omega} \omega]}{\partial Y} \Big|_{\eta} Y'} \\ \overline{L_k[X', Y']Y'|_{t=0}} &= \frac{\partial Y_0}{\partial \beta} \Big|_{\eta} \overline{L_k[X', Y']\beta'} \end{aligned}$$

Comparing these equations to the state representer equations (2.25), we see that the fact (2.34) holds if the following four identities hold.

$$\overline{L_k[X', Y']\alpha'} = C_\alpha \int_0^{t_f} \left(\left. \frac{\partial \phi}{\partial \alpha} \right|_\eta^T \Omega^k(t') + \left. \frac{\partial \varphi}{\partial \alpha} \right|_\eta^T \Lambda^k(t') \right) dt' \quad (\text{A.3})$$

$$\overline{L_k[X', Y']D_\nu P_\nu \nu} = \int_0^{t_f} D_\nu P_\nu C_\nu(t, t') P_\nu^T D_\nu^T \Omega^k(t') dt' \quad (\text{A.4})$$

$$\overline{L_k[X', Y']D_\omega(Y^\eta)P_\omega \omega} = \int_0^{t_f} D_\omega(Y^\eta(t)) P_\omega C_\omega(t, t') P_\omega^T [D_\omega(Y^\eta(t'))]^T \Lambda^k(t') dt' \quad (\text{A.5})$$

$$\overline{L_k[X', Y']\beta'} = C_\beta \left. \frac{\partial Y_0}{\partial \beta} \right|_\eta^T \Lambda^k|_{t=0} \quad (\text{A.6})$$

For the proof of (A.3)–(A.6) we seek an expression of the form

$$L_k[X', Y'] \approx \delta M_k[X, Y] = \frac{\delta M_k}{\delta X} \delta X + \frac{\delta M_k}{\delta Y} \delta Y = \frac{\delta M_k}{\delta \nu} \delta \nu + \frac{\delta M_k}{\delta \omega} \delta \omega + \frac{\delta M_k}{\delta \alpha} \delta \alpha + \frac{\delta M_k}{\delta \beta} \delta \beta$$

To this end, we apply an adjoint technique which avoids the explicit computation of $\frac{\delta M_k}{\delta X}$ and $\frac{\delta M_k}{\delta Y}$ and yields the derivatives with respect to ν , ω , α , and β directly. We first define as an objective the function for which we need the derivatives.

$$\tilde{J}^k = M_k[\bar{X}^{\eta+1}, \bar{Y}^{\eta+1}] + L_k[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] \quad (\text{A.7})$$

In order to satisfy the relation between the states X , Y and the inputs ν , ω , α , and β , we adjoin the tangent-linear state equation (2.13) to the objective.

$$\begin{aligned} J^k &= M_k[\bar{X}^{\eta+1}, \bar{Y}^{\eta+1}] + L_k[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] \\ &+ \int_0^{t_f} (\tilde{\mu}^k)^T \left(\phi(X^\eta, Y^\eta; \alpha^\eta) + \left. \frac{\partial \phi}{\partial X} \right|_\eta (X - X^\eta) + \left. \frac{\partial \phi}{\partial Y} \right|_\eta (Y - Y^\eta) \right. \\ &\quad \left. + \left. \frac{\partial \phi}{\partial \alpha} \right|_\eta (\alpha - \alpha^\eta) + D_\nu P_\nu \nu \right) dt \\ &- \int_0^{t_f} (\tilde{\lambda}^k)^T \left(\frac{\partial Y}{\partial t} - \varphi(X^\eta, Y^\eta; \alpha^\eta) - \left. \frac{\partial \varphi}{\partial X} \right|_\eta (X - X^\eta) - \left. \frac{\partial \varphi}{\partial Y} \right|_\eta (Y - Y^\eta) - \left. \frac{\partial \varphi}{\partial \alpha} \right|_\eta (\alpha - \alpha^\eta) \right. \\ &\quad \left. - D_\omega(Y^\eta) P_\omega \omega - \left. \frac{\partial [D_\omega(Y) P_\omega \omega]}{\partial Y} \right|_\eta (Y - Y^\eta) \right) dt \\ &\quad - (\tilde{\lambda}_0^k)^T \left(Y|_{t=0} - Y_0(\beta^\eta) - \left. \frac{\partial Y_0}{\partial \beta} \right|_\eta (\beta - \beta^\eta) \right) \quad (\text{A.8}) \end{aligned}$$

Using partial integration we substitute

$$- \int_0^{t_f} (\tilde{\lambda}^k)^T \frac{\partial Y}{\partial t} dt = + \int_0^{t_f} \frac{\partial \tilde{\lambda}^k}{\partial t} Y dt - ((\tilde{\lambda}^k)^T Y)|_{t=t_f} + ((\tilde{\lambda}^k)^T Y)|_{t=0}$$

in (A.8) and then use the resulting expression to compute the first variation of J^k .

$$\delta J^k = \frac{\delta J^k}{\delta X} \delta X + \frac{\delta J^k}{\delta Y} \delta Y + \frac{\delta J^k}{\delta \nu} \delta \nu + \frac{\delta J^k}{\delta \omega} \delta \omega + \frac{\delta J^k}{\delta \alpha} \delta \alpha + \frac{\delta J^k}{\delta \beta} \delta \beta \quad (\text{A.9})$$

We now choose $\tilde{\mu}^k$, $\tilde{\lambda}^k$ and $\tilde{\lambda}_0^k$ such that $\frac{\delta J^k}{\delta X} \delta X \equiv \frac{\delta J^k}{\delta Y} \delta Y \equiv 0$, because then we have

$$\delta J^k = \delta \tilde{J}^k \equiv \delta L_k[X, Y] = L_k[X', Y'] \quad (\text{A.10})$$

First, the variation of J^k with respect to X and Y yields

$$\begin{aligned} \frac{\delta J^k}{\delta X} \delta X &= \int_0^{t_f} \left(\delta(t - t_k) \frac{\partial f_k}{\partial X} \Big|_{\eta} + (\tilde{\mu}^k)^T \frac{\partial \phi}{\partial X} \Big|_{\eta} + (\tilde{\lambda}^k)^T \frac{\partial \varphi}{\partial X} \Big|_{\eta} \right) \delta X dt = 0 \\ \frac{\delta J^k}{\delta Y} \delta Y &= \int_0^{t_f} \left(\delta(t - t_k) \frac{\partial f_k}{\partial Y} \Big|_{\eta} + (\tilde{\mu}^k)^T \frac{\partial \phi}{\partial Y} \Big|_{\eta} + \frac{\partial \tilde{\lambda}^k}{\partial t} + (\tilde{\lambda}^k)^T \frac{\partial \varphi}{\partial Y} \Big|_{\eta} \right. \\ &\quad \left. + (\tilde{\lambda}^k)^T \frac{\partial [D_\omega(Y) P_\omega \omega]}{\partial Y} \Big|_{\eta} \right) \delta Y dt = 0 \end{aligned} \quad (\text{A.11})$$

as well as $\tilde{\lambda}_0^k = \tilde{\lambda}^k|_{t=0}$ and $\tilde{\lambda}^k|_{t=t_f} = 0$. Comparing (A.11) with the adjoint representation equations (2.24), we see that $\tilde{\mu}^k$ and $\tilde{\lambda}^k$ obey the same equations as Ω^k and Λ^k and therefore $\tilde{\mu}^k \equiv \Omega^k$ and $\tilde{\lambda}^k \equiv \Lambda^k$.

The other variations of J^k yield

$$\begin{aligned} \frac{\delta J^k}{\delta \nu} \delta \nu &= \int_0^{t_f} (\tilde{\mu}^k)^T D_\nu P_\nu \delta \nu dt \\ \frac{\delta J^k}{\delta \omega} \delta \omega &= \int_0^{t_f} (\tilde{\lambda}^k)^T D_\omega(Y^\eta) P_\omega \delta \omega dt \\ \frac{\delta J^k}{\delta \alpha} \delta \alpha &= \int_0^{t_f} \left((\tilde{\mu}^k)^T \frac{\partial \phi}{\partial \alpha} \Big|_{\eta} + (\tilde{\lambda}^k)^T \frac{\partial \varphi}{\partial \alpha} \Big|_{\eta} \right) \delta \alpha dt \\ \frac{\delta J^k}{\delta \beta} \delta \beta &= (\tilde{\lambda}_0^k)^T \frac{\partial Y_0}{\partial \beta} \Big|_{\eta} \delta \beta \end{aligned}$$

Using $\tilde{\mu}^k \equiv \Omega^k$, $\tilde{\lambda}^k \equiv \Lambda^k$ and the fact that $L_k[X', Y']$ is a scalar (for example $\frac{\delta J^k}{\delta \omega} \delta \omega = \delta \omega^T \frac{\delta J^k}{\delta \omega}$), we can now write $L_k[X', Y']$ according to (A.9) and (A.10) as

$$\begin{aligned} L_k[X', Y'] &= \int_0^{t_f} \delta \nu^T P_\nu^T D_\nu^T \Omega^k dt + \int_0^{t_f} \delta \omega^T P_\omega^T [D_\omega(Y^\eta)]^T \Lambda^k dt \\ &\quad + \int_0^{t_f} \delta \alpha^T \left(\frac{\partial \phi}{\partial \alpha} \Big|_{\eta}^T \Omega^k + \frac{\partial \varphi}{\partial \alpha} \Big|_{\eta}^T \Lambda^k \right) dt + \delta \beta^T \frac{\partial Y_0}{\partial \beta} \Big|_{\eta}^T \Lambda^k|_{t=0} \end{aligned}$$

If we left-multiply this expression with $\delta\alpha \equiv \alpha'$, take the expectation, and keep in mind that the cross-covariances (2.4a) between α and ν , ω or β vanish, we find (A.3). Similarly, multiplication with ν , ω , and β' yield (A.5), (A.4), and (A.6). This completes our proof of (2.34).

A.2.2 Derivation of the Posterior Covariance Equations

Before we start with the derivation of the posterior covariances, we prove the following result. Whereas the representer functions are deterministic, the representer coefficients are random variables. Their covariance is

$$\overline{b_k b_l} = [U^{-1}]_{kl} \quad (\text{A.12})$$

where we defined earlier

$$U \equiv C_v + R \quad \text{and} \quad [R]_{kl} \equiv L_k[\Xi^l, \Upsilon^l] \quad (\text{2.27})$$

This result is easily derived from (2.26). We have

$$\begin{aligned} \overline{b_k b_l} &= \sum_{rs} [U^{-1}]_{kr} \overline{(Z_r - M_r[X^\eta, Y^\eta] - L_r[\bar{X}^{\eta+1} - X^\eta, \bar{Y}^{\eta+1} - Y^\eta])} \\ &\quad \cdot \overline{(Z_s - M_s[X^\eta, Y^\eta] - L_s[\bar{X}^{\eta+1} - X^\eta, \bar{Y}^{\eta+1} - Y^\eta])} [U^{-1}]_{sl} \\ &= \sum_{rs} [U^{-1}]_{kr} (v_r + L_r[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]) (v_s + L_s[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]) [U^{-1}]_{sl} \\ &= \sum_{rs} [U^{-1}]_{kr} \left([C_v]_{rs} + \overline{L_r[X', Y'] L_s[X', Y']} \right) [U^{-1}]_{sl} \end{aligned}$$

With $\overline{L_r[X', Y'] L_s[X', Y']} = L_r[\overline{L_s[X', Y'] X'}, \overline{L_s[X', Y'] Y'}] = L_r[\Xi^s, \Upsilon^s] = R_{rs}$, the desired result follows immediately.

We are now finally ready to derive the equations (2.35), (2.36), and (2.37) for the posterior covariances. Using the previous results, the derivations are straightforward. First, we expand the expression for the posterior state covariance $C_{\tilde{Y}\tilde{Y}}$.

$$\begin{aligned} [C_{\tilde{Y}\tilde{Y}}(t_1, t_2)]_{ij} &\equiv \overline{(Y_i(t_1) - Y_i^{\eta+1}(t_1))(Y_j(t_2) - Y_j^{\eta+1}(t_2))} \\ &= \overline{(Y_i(t_1) - \bar{Y}_i^{\eta+1}(t_1) - \sum_k b_k \Upsilon_i^k(t_1))(Y_j(t_2) - \bar{Y}_j^{\eta+1}(t_2) - \sum_l b_l \Upsilon_j^l(t_2))} \\ &= [C_{Y'Y'}(t_1, t_2)]_{ij} - \sum_k \Upsilon_i^k(t_1) \overline{b_k (Y_j(t_2) - \bar{Y}_j^{\eta+1}(t_2))} \\ &\quad - \sum_l \Upsilon_j^l(t_2) \overline{b_l (Y_i(t_1) - \bar{Y}_i^{\eta+1}(t_1))} + \sum_{kl} \Upsilon_i^k(t_1) \overline{b_k b_l} \Upsilon_j^l(t_2) \end{aligned}$$

Using (A.12) and

$$\begin{aligned}
& \overline{b_k(Y_j(t_2) - \bar{Y}_j^{\eta+1}(t_2))} \\
&= \sum_r [U^{-1}]_{kr} \overline{(Z_r - M_r[X^\eta, Y^\eta] - L_r[\bar{X}^{\eta+1} - X^\eta, \bar{Y}^{\eta+1} - Y^\eta])(Y_j(t_2) - \bar{Y}_j^{\eta+1}(t_2))} \\
&= \sum_r [U^{-1}]_{kr} \overline{(v_r + L_r[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}])(Y_j(t_2) - \bar{Y}_j^{\eta+1}(t_2))} \\
&= \sum_r [U^{-1}]_{kr} \overline{L_r[X', Y']Y_j'(t_2)} \\
&= \sum_r [U^{-1}]_{kr} \Upsilon_j^r(t_2)
\end{aligned}$$

we immediately get the corresponding equation in (2.35). The other posterior state covariance equations of can be derived analogously.

In order to derive the posterior covariance of the measurement predictions (2.36), we expand

$$\begin{aligned}
[C_{\bar{v}}]_{mn} &\equiv \overline{L_m[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} \\
&= \overline{(L_m[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] - \sum_k b_k L_m[\Xi^k, \Upsilon^k])} \\
&\quad \cdot \overline{(L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] - \sum_l b_l L_n[\Xi^l, \Upsilon^l])} \\
&= \overline{L_m[X', Y']L_n[X', Y']} - \sum_k L_m[\Xi^k, \Upsilon^k] \overline{b_k L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} \\
&\quad - \sum_l L_n[\Xi^l, \Upsilon^l] \overline{b_l L_m[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} + \sum_{kl} L_m[\Xi^k, \Upsilon^k] \overline{b_k b_l} L_n[\Xi^l, \Upsilon^l]
\end{aligned}$$

With $L_m[\Xi^k, \Upsilon^k] = R_{mk}$ and

$$\begin{aligned}
& \overline{b_k L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} \\
&= \sum_l [U^{-1}]_{kl} \overline{(Z_l - M_l[X^\eta, Y^\eta] - L_l[\bar{X}^{\eta+1} - X^\eta, \bar{Y}^{\eta+1} - Y^\eta])L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} \\
&= \sum_l [U^{-1}]_{kl} \overline{(v_l + L_l[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}])L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]} \\
&= \sum_l [U^{-1}]_{kl} \overline{L_l[X', Y']L_n[X', Y']} \\
&= \sum_l [U^{-1}]_{kl} R_{ln}
\end{aligned}$$

we immediately obtain (2.36).

Finally, for the covariance of the posterior data residuals (2.37) we expand

$$\begin{aligned}
[C_{\hat{v}}]_{mn} &\equiv \overline{(Z_m - M_m[X^\eta, Y^\eta] - L_m[X^{\eta+1} - X^\eta, Y^{\eta+1} - Y^\eta]) \cdot (Z_n - M_n[X^\eta, Y^\eta] - L_n[X^{\eta+1} - X^\eta, Y^{\eta+1} - Y^\eta])} \\
&= \overline{(v_m + L_m[X - X^{\eta+1}, Y - Y^{\eta+1}]) (v_n + L_n[X - X^{\eta+1}, Y - Y^{\eta+1}])} \\
&= \overline{(v_m + L_m[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] - \sum_k b_k L_m[\Xi^k, \Upsilon^k]) \cdot (v_n + L_n[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}] - \sum_l b_l L_n[\Xi^l, \Upsilon^l])} \\
&= \overline{v_m v_n} - \sum_l L_n[\Xi^l, \Upsilon^l] \overline{b_l v_m} - \sum_k L_m[\Xi^k, \Upsilon^k] \overline{b_k v_n} + [C_{\hat{v}}]_{mn}
\end{aligned}$$

Using $L_n[\Xi^l, \Upsilon^l] = R_{nl}$ and

$$\begin{aligned}
\overline{b_l v_m} &= \sum_r [U^{-1}]_{lr} \overline{(Z_r - M_r[X^\eta, Y^\eta] - L_r[\bar{X}^{\eta+1} - X^\eta, \bar{Y}^{\eta+1} - Y^\eta]) v_m} \\
&= \sum_r [U^{-1}]_{lr} (v_r + L_r[X - \bar{X}^{\eta+1}, Y - \bar{Y}^{\eta+1}]) v_m \\
&= \sum_r [U^{-1}]_{lr} [C_v]_{rm}
\end{aligned}$$

we get

$$\begin{aligned}
[C_{\hat{v}}]_{mn} &= [C_v]_{mn} - \sum_{lr} R_{nl} [U^{-1}]_{lr} [C_v]_{rm} - \sum_{ks} R_{mk} [U^{-1}]_{ks} [C_v]_{sn} + [C_{\hat{v}}]_{mn} \\
&= [C_v]_{mn} - [RU^{-1}C_v]_{nm} - [RU^{-1}C_v]_{mn} + [C_{\hat{v}}]_{mn}
\end{aligned}$$

which is obviously (2.37).

Appendix B

Land Surface Model

B.1 List of Symbols

Tables B.1 to B.8 provide a list of all symbols used in the land surface model. The last column generally indicates in which spatial dimensions the variables or parameters vary and whether they are time-dependent. First, a list of the state and observation variables is shown in Table B.1. The three state variables for soil moisture can be used interchangeably. They are connected through the Clapp-Hornberger relations (3.4). The soil moisture and temperature states and the interception water are governed by ODE's, therefore initial conditions must be specified.

Next, Table B.2 lists the meteorologic inputs to the model. Tables B.3 and B.4 compile all the time-dependent variables and parameters. The functional dependence is indicated. Note that empirical and physical constants are not listed in this functional dependence. Tables B.5 and B.6 list the time-independent parameters, most of which must be specified as model inputs. Table B.7 contains all the scalar empirical constants with their values or appropriate references. Finally, Table B.8 shows all the physical constants in the model. Those numbers are fixed and never used for calibration.

Recall the notational convention to label most of the empirical constants in the various parameterizations with κ for scalar constants and with β for distributed parameters (which for example depend on texture or vegetation). The empirical parameters are superscripted with the variable which is being parameterized and subscripted with a number in case more than one empirical constant is needed.

Moreover, the subscripts r, a, c, g refer to **r**eference (or screen) height, **a**ir (within the canopy), **c**anopy (plant material), and **g**round, respectively. Note that all variables at screen height are inputs that are directly measured or derived from meteorologic observations. The subscripts s and l are used for **s**hortwave and **l**ongwave, s and u are used for **s**aturated and **u**nsaturated, depending on context. The symbol f always denotes a fraction varying from 0 to 1.

Lastly, in our convention the matric head ψ_g is negative for unsaturated conditions. The vertical coordinate z is positive upward, and the numbering of the layers increases upward.

Symbol	Units	Description	Dimension
W_g	$[-]$	soil wetness/saturation	x, y, z, t
θ_g	$[m^3/m^3]$	volumetric soil moisture content	
ψ_g	$[m]$	matric head	
T_g	$[K]$	soil surface temperature	x, y, t
W_c	$[m]$	canopy interception water	x, y, t
T_c	$[K]$	canopy temperature	x, y, t
e_a	$[mb]$	canopy air vapor pressure	x, y, t
T_a	$[K]$	canopy air temperature	x, y, t
T_B	$[K]$	radiobrightness temperature	x, y, t

Table B.1: State variables of the land surface model.

Symbol	Units	Description	Dimension
P_r	$[m/s]$	precipitation at ref. height	x, y, t
R_{rs}	$[W/m^2]$	incoming shortw. radiation at ref. height	x, y, t
T_r	$[K]$	atmospheric temperature at ref. height	x, y, t
e_r	$[mb]$	vapor pressure at ref. height	x, y, t
u_r	$[m/s]$	wind speed at ref. height	x, y, t
T_d	$[K]$	depth average soil temperature	$x, y, (t)$

Table B.2: Meteorologic inputs. The depth average soil temperature changes on a seasonal time-scale only.

Sym.	Units	Description	Dependency	Dim.
P_t	$[m/s]$	throughfall rate of precipitation	$P_t(P_r, P_i, D_c, f_c)$	x, y, t
P_i	$[m/s]$	interception rate of precipitation	$P_i(P_r, W_c, W_c^{\max})$	x, y, t
D_c	$[m/s]$	dripping rate from interception storage	$D_c(W_c, t_c^{\text{drip}})$	x, y, t
S_g	$[1/s]$	root sink term for transp. loss	$S_g(E_{ct}^{\text{pot}}, \chi_g(W_g))$	x, y, z, t
G_g	$[W/m^2]$	ground heat flux	$G_g(R_{gs}^{\text{net}}, R_{gl}^{\text{net}}, E_g, H_g)$	x, y, t
R_{rl}	$[W/m^2]$	incoming longw. radiation at ref. height	$R_{rl}(T_r, \epsilon_r)$	x, y, t
R_{gs}^{net}	$[W/m^2]$	net shortw. radiation at ground surface	$R_{gs}^{\text{net}}(R_{rs}, a_g, f_c)$	x, y, t
R_{gl}^{net}	$[W/m^2]$	net longw. radiation at ground surface	$R_{gl}^{\text{net}}(R_{rl}, T_g, T_c, \epsilon_g, \epsilon_c, f_c)$	x, y, t
R_{cs}^{net}	$[W/m^2]$	net shortw. radiation at canopy	$R_{cs}^{\text{net}}(R_{rs}, a_c, f_c)$	x, y, t
R_{cl}^{net}	$[W/m^2]$	net longw. radiation at canopy	$R_{cl}^{\text{net}}(R_{rl}, T_g, T_c, \epsilon_g, \epsilon_c, f_c)$	x, y, t
a_g	$[-]$	ground surface albedo	$a_g(W_g, \theta_s)$	x, y, t
ϵ_g	$[-]$	longw. soil surface emissivity	$\epsilon_g(W_g)$	x, y, t
ϵ_r	$[-]$	longw. atmospheric emissivity	$\epsilon_r(e_r)$	x, y, t
E_a	$[kg/m^2/s]$	evapotransp. rate to atmosphere	$E_a(e_a, e_r, r_a)$	x, y, t
E_g	$[kg/m^2/s]$	ground surface evap. rate	$E_g(e_s(T_g), e_a, r_g, r_d, f_c)$	x, y, t
E_{ce}	$[kg/m^2/s]$	(wet) canopy evap. rate	$E_{ce}(e_s(T_c), e_a, r_c, r_s, \text{LSAI}, f_c, f_{ce})$	x, y, t
E_{ct}^{pot}	$[kg/m^2/s]$	potential (dry) canopy transp. rate	$E_{ct}^{\text{pot}}(e_s(T_c), e_a, r_c, r_s, \text{LAI}, f_c, f_{ce})$	x, y, t
E_{ct}	$[kg/m^2/s]$	actual (dry) canopy transp. rate	$E_{ct}(E_{ct}^{\text{pot}}, \chi_g(W_g))$	x, y, t
H_a	$[W/m^2]$	sensible heat flux to atmosphere	$H_a(T_r, T_a, r_a)$	x, y, t
H_g	$[W/m^2]$	sensible heat flux at ground surface	$H_g(T_g, T_a, r_d, f_c)$	x, y, t
H_c	$[W/m^2]$	sensible heat flux from canopy	$H_c(T_c, T_a, r_c, \text{LSAI}, f_c)$	x, y, t
e_s	$[mb]$	saturation vapor pressure	$e_s(T)$	x, y, t
u_c	$[m/s]$	wind speed at canopy height	$u_c(u_r, z_r, z_0, d_c, h_c)$	x, y, t
u_*	$[m/s]$	friction velocity	$u_*(u_r, z_r, z_0, d_c)$	x, y, t
r_a	$[s/m]$	atmospheric resistance	$r_a(u_r, z_r, z_0, d_c)$	x, y, t
r_c	$[s/m]$	bulk canopy resistance	$r_c(u_c)$	x, y, t
r_d	$[s/m]$	aerodynamic resistance within canopy	$r_d(u_c)$	x, y, t
r_g	$[s/m]$	surface resistance of bare soil	$r_g(W_g, \theta_s)$	x, y, t
r_s	$[s/m]$	stomatal resistance	$r_s(r_s^{\min}, \chi_c(R_{rs}))$	x, y, t
C_g	$[J/m^3/K]$	vol. heat capacity of wet top soil layer	$C_g(\rho_{gb}, c_g, W_g, \theta_s)$	x, y, t
λ_g	$[W/m/K]$	thermal conductivity of wet top soil layer	$\lambda_g(W_g, \theta_s)$	x, y, t
q_t	$[m/s]$	moisture flux b.c. at top	$q_t(P_t, E_g)$	x, y, t
q_b	$[m/s]$	moisture flux b.c. at bottom	$q(K_u)$	x, y, t
K_u	$[m/s]$	unsaturated hydraulic conductivity	$K_u(K_s, W_g)$	x, y, z, t
f_{ce}	$[-]$	wet canopy fraction (for canopy evap.)	$f_{ce}(W_c, W_c^{\max})$	x, y, t
χ_g	$[-]$	stress function for water-limited transp.	$\chi_g(W_g, \psi^{\text{wilt}}, f_R)$	x, y, z, t
χ_c	$[-]$	solar radiation influence on transp.	$\chi_c(R_{rs})$	x, y, t

Table B.3: Forcing variables and time-dependent parameters for the land surface model. Note that we assume the soil thermal diffusivity K_T to be constant in time (Section 3.1.7).

Symbol	Units	Description	Dependency	Dim.
k_g	$[-]$	microw. dielectric constant of wet soil	$k_g(W_g, \theta_s, k_w, k_{gd}, f_S, f_C)$	x, y, t
k_w	$[-]$	microw. dielectric constant of water	$k_w(k_{w0}, k_{w\infty}, \nu_r, \tau_w)$	x, y, t
k_{w0}	$[-]$	static dielectric constant of water	$k_{w0}(T_g)$	x, y, t
τ_w	$[s]$	relaxation time of water	$\tau_w(T_g)$	x, y, t
ε_{gp}	$[-]$	rough surface microw. emissivity for polariz. p	$\varepsilon_{gp}(k_g, \phi_r)$	x, y, t
$\varepsilon_{gp}^{\text{smooth}}$	$[-]$	smooth surface microw. emissivity for polariz. p	$\varepsilon_{gp}^{\text{smooth}}(k_g, \phi_r)$	x, y, t
T_g^{eff}	$[K]$	eff. soil temp. for microw. emission	$T_g^{\text{eff}}(T_g, k_g)$	x, y, t
ϕ_g	$[rad]$	in-soil propagation angle	$\phi_g(k_g, \phi_r)$	x, y, t
z_{grad}	$[m]$	gradient RT effective depth	$z_{\text{grad}}(\alpha_e, \phi_g)$	x, y, t
α_e	$[1/m]$	microw. attenuation coefficient	$\alpha_e(k_g, \nu_r)$	x, y, t

Table B.4: Time-dependent variables and parameters for the Radiative Transfer model. Note that ϕ_g , z_{grad} , and α_e are part of the Gradient RT approximation and not used.

Symbol	Units	Description/Value	Model Input ?	Dim.
δ_g	[m]	depth of surface temp. layer	yes	-
Δ_i	[m]	depth of finite difference soil moisture layer i	yes	z
$\bar{\Delta}_i$	[m]	depth of layer “around” soil moisture node i	$\bar{\Delta}(\Delta)$	z
θ_s	[m^3/m^3]	porosity	yes	x, y, z
K_s	[m/s]	saturated hydraulic conductivity	yes	x, y, z
ψ^{CH}	[m]	[Clapp and Hornberger, 1978]	yes	x, y, z
B^{CH}	[-]	[Clapp and Hornberger, 1978]	yes	x, y, z
W^{r_g}	[-]	surface resistance param. (0.25 ... 0.6)	yes	x, y
r_g^{max}	[s/m]	surface resistance param. (3000 ... 7000)	yes	x, y
β^{r_g}	[-]	surface resistance param.	$\beta^{r_g}(W^{r_g}, r_g^{\text{max}})$	x, y
K_T	[m^2/s]	thermal diffusivity of soil surface layer	yes	x, y
d_g	[m]	damping depth of temp. forcing	$d_g(K_T)$	x, y
α_g	[-]	param. of force-restore approx.	$\alpha_g(d_g, \delta_g)$	x, y
Γ_g	[1/s]	coefficient in force-restore approx.	$\Gamma_g(\alpha_g)$	x, y
Γ'_g	[s/m]	coefficient in force-restore approx.	$\Gamma'_g(K_T)$	x, y
ρ_{gb}	[kg/m ³]	bulk density of (dry) soil in layer δ_g	$\rho_{gb}(\theta_s, \rho_g)$	x, y
c_g	[J/kg/K]	specific heat of dry soil in layer δ_g	yes	x, y
z_r	[m]	reference (or screen) height	yes	-
h_c	[m]	vegetation height (also for bare soil z_0)	yes	$x, y, (t)$
d_c	[m]	zero plane displacement height	$d_c(h_c)$	$x, y, (t)$
z_0	[m]	roughness length	$z_0(h)$	$x, y, (t)$
β^{r_c}	[$\sqrt{s/m}$]	[Sellers and Dorman, 1987]	yes	$x, y, (t)$
β^{r_d}	[-]	[Sellers and Dorman, 1987]	yes	$x, y, (t)$
r_s^{min}	[s/m]	minimum stomatal resistance	yes	$x, y, (t)$
a_c	[-]	shortw. canopy albedo	yes	$x, y, (t)$
ϵ_c	[-]	longw. canopy emissivity	yes	$x, y, (t)$
W_c^{max}	[m]	max intercepted water	$W_c^{\text{max}}(\text{LSAI})$	$x, y, (t)$
t_c^{drip}	[s]	dripping time for canopy interception storage	yes	$x, y, (t)$
f_c	[-]	area fraction shaded by vegetation canopy	yes	$x, y, (t)$
ψ^{wilt}	[m]	wilting point	yes	$x, y, (t)$
d_R	[m]	typical rooting depth	yes	$x, y, (t)$
ρ_R	[1/m]	root density distribution	$\rho_R(d_R)$	$x, y, z, (t)$
f_R	[-]	root distribution factor	$f_R(d_R)$	$x, y, z, (t)$
LAI	[-]	(green) leaf area index	yes	$x, y, (t)$
SAI	[-]	stem (and dead leaf) area index	yes	$x, y, (t)$
LSAI	[-]	leaf and stem area index	LSAI(LAI, SAI)	$x, y, (t)$
$\beta_1^{\lambda_g}$	[W/m/K]	-0.197 (clay), 0.243 (loam), 0.228 (sand)	(yes)	x, y
$\beta_2^{\lambda_g}$	[W/m/K]	-0.962 (clay), 0.393 (loam), -2.406 (sand)	(yes)	x, y
$\beta_3^{\lambda_g}$	[W/m/K]	2.521 (clay), 1.534 (loam), 4.909 (sand)	(yes)	x, y

Table B.5: Time-independent parameters for the land surface model. Note that we assume the soil thermal diffusivity K_T to be a constant in time (Section 3.1.7), that is the $\beta_i^{\lambda_g}$ are not used. Note also that vegetation parameters are time-dependent on the time-scale of plant growth, which is indicated by (t) .

Symbol	Units	Description	Model Input ?	Dim.
ν_r	[Hz]	microw. observation frequency	yes	-
ϕ_r	[rad]	(in-air) look-angle from nadir at ref. height	yes	-
f_S	[-]	sand fraction in layer δ_g	yes	x, y
f_C	[-]	clay fraction in layer δ_g	yes	x, y
β^{k_g}	[-]	Dobson dielectric mixing model param.	$\beta^{k_g}(f_S, f_C)$	x, y
β^{e_g}	[-]	surface roughness param. [Choudhury et al., 1979]	yes	x, y
W_v	[kg/m ²]	vegetation water content	yes	$x, y, (t)$
β^{δ_c}	[m ² /kg]	“vegetation b param.” [Jackson and Schmugge, 1991]	yes	$x, y, (t)$
δ_c	[-]	canopy optical depth	$\delta_c(W_v, \phi_r)$	$x, y, (t)$
α_c	[-]	canopy microwave attenuation	$\alpha_c(\delta_c)$	$x, y, (t)$
z_{grey}	[m]	grey body RT param.	yes	-

Table B.6: Time-independent parameters for the Radiative Transfer model. Note that vegetation parameters are time-dependent on the time-scale of plant growth, which is indicated by (t) .

Symbol	Value	Units
$\kappa_1^{u_g}$	0.25	[-]
$\kappa_2^{u_g}$	0.125	[-]
$\kappa_1^{e_r}$	0.74	[-]
$\kappa_2^{e_r}$	0.0049	[-]
$\kappa_1^{e_g}$	0.9	[-]
$\kappa_2^{e_g}$	0.18	[-]
κ^{r_g}	10	[s/m]
$\kappa_1^{\alpha_g}$	0.943	[-]
$\kappa_2^{\alpha_g}$	0.223	[-]
$\kappa_3^{\alpha_g}$	$1.68 \cdot 10^{-2}$	[-]
$\kappa_4^{\alpha_g}$	$-5.27 \cdot 10^{-3}$	[-]
κ^{d_c}	0.63	[-]
κ^{z_0}	0.13	[-]
κ^{W_c}	$10^{-4} \dots 10^{-3}$	[m]
$\kappa_1^{\chi_c}$	50 ... 100	[-]
$\kappa_2^{\chi_c}$	100 ... 200	[W/m ²]
$\kappa^{J_{ce}}$	2/3	[-]
$\kappa_1^{k_g}$	0.65	[-]
$\kappa_2^{k_g}$	1.09	[-]
$\kappa_3^{k_g}$	0.11	[-]
$\kappa_4^{k_g}$	-0.18	[-]
$\kappa_1^{k_{w0}}$	88.045	[-]
$\kappa_2^{k_{w0}}$	-0.4147	[1/K]
$\kappa_3^{k_{w0}}$	$6.295 \cdot 10^{-4}$	[1/K ²]
$\kappa_4^{k_{w0}}$	$1.075 \cdot 10^{-5}$	[1/K ³]
$\kappa_1^{\tau_{w0}}$	$1.1109 \cdot 10^{-10}$	[s]
$\kappa_2^{\tau_{w0}}$	$-3.824 \cdot 10^{-12}$	[s/K]
$\kappa_3^{\tau_{w0}}$	$6.938 \cdot 10^{-14}$	[s/K ²]
$\kappa_4^{\tau_{w0}}$	$-5.096 \cdot 10^{-16}$	[s/K ³]
C_{grad}	1.03	[-]

Table B.7: Scalar empirical constants.

Symbol	Value	Units	Description
ρ_w	1000	$[kg/m^3]$	density of water
ρ_a	1.20	$[kg/m^3]$	density of air
ρ_g	$2.65 \cdot 10^3$	$[kg/m^3]$	density of soil particles in layer δ_g
ω_d	$2\pi/86400$	$[1/s]$	angular frequency of diurnal cycle
L	$2.5 \cdot 10^6$	$[J/kg]$	latent heat of vaporization
σ	$5.57 \cdot 10^{-8}$	$[W/m^2/K^4]$	Stefan-Boltzmann constant
γ	0.65	$[mb/K]$	psychrometric constant
c_a	1004	$[J/kg/K]$	specific heat of air at constant pressure
c_w	4187	$[J/kg/K]$	specific heat of water
K	0.4	$[-]$	von Karman constant
T_0	273.15	$[K]$	reference temperature
k_{gd}	4.67	$[-]$	microw. dielectric constant of dry soil
$k_{w\infty}$	4.9	$[-]$	high frequency dielectric constant of water
g	9.81	$[m/s^2]$	acceleration due to gravity
c_{light}	$3 \cdot 10^8$	$[m/s]$	speed of light

Table B.8: Physical constants

